Wrapping Current versus Bulk Integer Quantum Hall Effect in Three Dimensions

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Surface electron currents are studied for the integer quantum Hall effect in three dimensions(3D) proposed previously by Kohmoto et al. and by Koshino et al. We predict the current wraps the facets of the sample with its intensity and direction dictated by 3D Chern numbers which are just the quantized Hall conductivities in 3D (σ_{xy}, σ_{zx}), so a natural connection exists between the surface and bulk currents just as in 2D. An experiment to detect the 3D integer quantum Hall effect through the wrapping current is proposed.

The chiral edge states of 2D electrons in magnetic fields have been extensively investigated for the quantum Hall effect(QHE)[1]. Namely, edge states exist for each Landau gap in a finite quantum Hall system, and the Hall current carried by them is shown to coincide exactly with one calculated with the Kubo formula[2] for the bulk sample, which has been interpreted in terms of topological quantum numbers characterizing the quantum Hall currents[3].

While the QHE is usually conceived as specific to two-dimensional systems, it is known that integer QHE can occur even in three dimensions (3D) if the spectrum has an energy gap and if the Fermi energy lies in the gap[4–6]. Although gaps do not usually appear in 3D, two of the present authors have shown[7] that it is possible to have a class of energy spectra having a series of gaps (Hofstadter butterfly) in 3D lattice systems in an appropriate condition, where we have a 3D-specific IQHE, i.e., each of the Hall conductivities σ_{xy}, σ_{zx} quantized for each gap. That analysis for the 3D QHE is based on the bulk description, and a natural question we can now ask is: whether and how surface states appear in this 3D QHE. In superlattice systems, i.e., stack of 2D systems, the surface current has been intensively studied.[8] There, one discusses a stack of the chiral edge states, called the chiral sheath current. Surface states are also discussed for the field-induced spin density waves (FISDW) in organic conductors[9,10]. In those systems, however, the inter-layer hoppings are relatively so small that the surface states may be understood as weakly coupled 2D edge states. By contrast, here we are talking about the 3D-specific IQHE with σ_{xy}, σ_{zx} quantized as 3D Chern (topological) numbers.

So we have studied here the surface states for 3D in general and for the 3D butterfly in particular. We show that there exists a surface *wrapping current* that winds around the facets of the 3D sample. A hallmark of the 3D-specific nature appears as the current on each facet flowing obliquely to the crystallographic axes, where the current direction is given in terms of the 3D Chern numbers. An interesting observation is that the 3D Hall currents carried by surface states are exactly the same as what is given by the bulk conductivities.
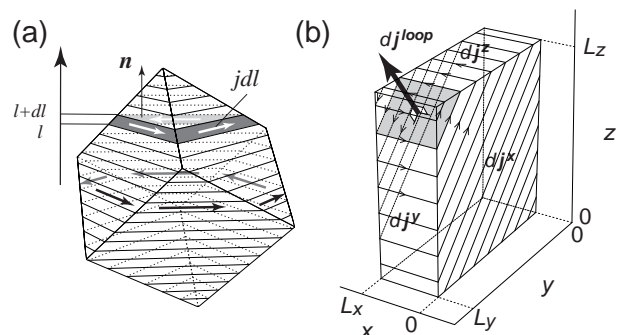

FIG. 1. (a)A schematic picture of the surface wrapping current. $\boldsymbol{j}^{\mathrm{loop}} = j\boldsymbol{n}$ is the surface loop current density. (b)The wrapping current calculated for the microscopic model for the 3D QHE case (eqs.(11) and (14)).

Although we can expect a 3D sample in a magnetic field spontaneously carries a surface current in equilibrium as a 2D sample carries an edge current, the situation should be more complex, since the surface current will have to wind around various faces of the 3D sample. However, we can show, from thermodynamics, that the surface current may be expressed in a surprisingly simple way in terms of the bulk density of states. Let us take a cubic, homogeneous sample for simplicity and put it in a uniform magnetic field $\boldsymbol{B}$. We assume that the surface current is uniform over each face of the cube and that the effect of cube edges can be neglected. Then we can characterize the surface current flowing around the faces of the cube by regarding it as a bunch of loop-current segments as depicted in Fig.1(a). Since the current is assumed to be uniform on each face, the bunch is characterized by only two quantities: the vector $\boldsymbol{n}$, normal to each loop, and j, the loop current intensity flowing within a unit height measured along $\boldsymbol{n}$. If we define the loop current-density vector as $\boldsymbol{j}^{\mathrm{loop}} \equiv j\boldsymbol{n}$, the magnetization associated with the current is $\boldsymbol{m} = V\boldsymbol{j}^{\mathrm{loop}}$, where V is the sample volume. Combining with a thermodynamic Maxwell's relation, we obtain

$$\frac{d\boldsymbol{j}^{\mathrm{loop}}}{\partial \mu} = \frac{\partial \rho}{\partial \boldsymbol{B}}, \tag{1}$$

where ρ is the density of occupied states per unit volume and μ the chemical potential.

Now if we move on to the QHE case in the 3D periodic system, by assuming that the Fermi energy E_F lies in a gap of the bulk energy spectrum[5,6], we have a relation

$$\frac{\partial \rho}{\partial \boldsymbol{B}} = -\frac{e}{2\pi h}\boldsymbol{J}, \qquad (2)$$

where $-e$ is the charge of an electron and $\boldsymbol{J}$ is a reciprocal vector of the periodic potential. $\boldsymbol{J}$ depends on the gap in which E_F lies and gives the quantized 3D Hall conductance through

$$\sigma_{ij}^{\text{bulk}} = \frac{e^2}{2\pi h}\sum_k \epsilon_{ijk} J_k, \qquad (3)$$

where ϵ_{ijk} is the unit antisymmetric tensor. From eqs.(1) and (2), the surface loop current carried by the surface states between E and $E + d\mu$ is given as

$$d\boldsymbol{j}^{\text{loop}} = -\frac{e}{2\pi h}\boldsymbol{J}d\mu. \qquad (4)$$

From this we will conclude that there is a quantized wrapping current. Even at this stage, we can see a unique behavior: that the direction (in real space) of the surface current should always be perpendicular to a fixed reciprocal vector, which in general deviates from the symmetry axes of the crystal and also from $\boldsymbol{B}$, but which is solely determined by the gap in which E_F is located.
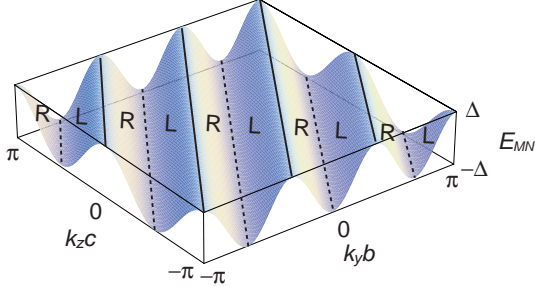

FIG. 2. The energy dispersion for the surface states on the $\hat{\boldsymbol{x}}$ faces in the energy gap $(M, N) = (3, 2)$. 'L' and 'R' represent the surface states on the left $(x = 0)$ and the right $(x = L_x)$ faces, respectively.

Having looked at the thermodynamics, let us move on to a microscopic model for the 3D QHE surface currents. We take a noninteracting tight-binding electron system in a uniform magnetic field $\boldsymbol{B}$. Schrödinger's equation is $-\sum_j t_{ij} e^{i\theta_{ij}} \psi_j = E\psi_i$. Here ψ_i is the wave function at site i, the summation is over nearest-neighbor sites, and $\theta_{ij} = \frac{e}{\hbar}\int_j^i \boldsymbol{A} \cdot d\boldsymbol{l}$ is the Peierls phase factor arising from the magnetic flux where $\boldsymbol{A}$ is the vector potential with $\nabla \times \boldsymbol{A} = \boldsymbol{B}$. We consider a 3D simple-cubic lattice with lattice constants a, b, c and $\boldsymbol{B} = (0, B\sin\theta, B\cos\theta)$ lying in the yz plane. In the gauge $\boldsymbol{A} = (0, Bx\cos\theta, -Bx\sin\theta)$, y, z become cyclic, and we

have $\psi_{lmn} = e^{ik_y mb + ik_z nc} F_l$, where l, m, n are the site indexes along x, y, z, respectively. Schrödinger's equation then reads

$$-t_x(F_{l-1} + F_{l+1}) - [2t_y \cos(G_b la + k_y b)$$
$$+2t_z \cos(-G_c la + k_z c)]F_l = EF_l. \qquad (5)$$

Here t_x, t_y, t_z are the transfer integrals between nearest neighbors along x, y, z, respectively, and $(G_b, G_c) = \frac{e}{\hbar}(B_z b, B_y c)$.

Now we consider that the system is quasi-1D, i.e., $t_x \gg t_y, t_z$, which is required for the 3D butterfly[7]. By applying the effective-mass approach for the x direction, we have

$$\big[E_x(\partial_x) - 2t_y \cos(G_b x + k_y b)$$
$$- 2t_z \cos(-G_c x + k_z c)\big]F(x) = EF(x), \qquad (6)$$

where $E_x(\partial_x) = (at_x \partial_x)^2$. The perturbation ($\propto t_y, t_z$) mixes eigenfunctions $\{F(x) = e^{ik_x x}\}$, and energy gaps of magnitude $\Delta = |t_y|^M |t_z|^N$ (in a unit of energy $t_x = 1$) open at $k_x = \pm\frac{1}{2}(MG_b + NG_c)$, where M, N are integers. In the quasi-1D limit $t_y, t_z \to 0$, Schrödinger's equation around the gap (M, N) simplifies into

$$\begin{pmatrix} -i\hbar v \partial_x & \Delta e^{i\varphi} \\ \Delta e^{-i\varphi} & i\hbar v \partial_x \end{pmatrix} \begin{pmatrix} F_+(x) \\ F_-(x) \end{pmatrix} = E \begin{pmatrix} F_+(x) \\ F_-(x) \end{pmatrix}, \qquad (7)$$

where we have decomposed the wave function into the left- and right-moving components, $F = F_+ + F_-$, around $k_x = \pm k_{\text{F}} = \pm\frac{1}{2}(MG_b + NG_c)$, $\varphi = Mk_y b - Nk_z c$, and $v = \hbar k_{\text{F}}/m^*$.

Now we consider the surface states at the gap (M, N) by extending the discussion for the FISDW[9,10], which is one way of realizing the energy gaps in 3D systems and also mathematically similar to the 3D QHE considered in ref.[7,11]. We first consider the surfaces normal to the conductive axis ($\hat{\boldsymbol{x}}$) in a sample with $0 \leq x \leq L_x$. By applying the boundary condition $F(0) = 0$ to the differential eq.(7), we find a surface state that decays into the bulk,

$$F(x) = e^{-\kappa x} \sin k_{\text{F}} x, \qquad (8)$$

where $\kappa = (\Delta/\hbar v) \sin(Mk_y b - Nk_z c)$. The corresponding eigenenergy measured from the gap center is

$$E_{MN} = -\Delta \cos(Mk_y b - Nk_z c). \qquad (9)$$

The solution with $\kappa > 0$ corresponds to the left surface ($x \simeq 0$) while $\kappa < 0$ to the right ($x \simeq L_x$). The energy dispersion of the surface state must be plotted against (k_y, k_z) as in Fig.2. They oscillate $M(N)$ times along $k_x(k_y)$, where we can see the stripe-like areas alternating for the right and left surface states. Since the Brillouin zone is topologically a torus, we can define two winding numbers for the stripe along toroidal and poloidal directions. They are just M and N, and these two numbers are in fact the Chern numbers in 3D, which correspond

to σ_{xy}, σ_{zx} as shown below. For 2D Hatsugai has shown that the edge states whose energy dispersions correspond to wiggly lines against k_y between the Landau subbands have topological numbers.[3] Hence the present result is a natural extension to 3D. Although small t_y, t_z are assumed above, the 3D Chern numbers, being topological, should be constant for larger t_y, t_z.

From this microscopic model, we can actually calculate the current density on the surface. The expected value of the velocity for the electron for given (k_y, k_z) is

$$\boldsymbol{v} = \frac{1}{\hbar}\frac{\partial E_{MN}}{\partial \boldsymbol{k}} = \pm\frac{1}{\hbar}\sqrt{\Delta^2 - E_{MN}^2}(0, Mb, -Nc), \quad (10)$$

where $+$ and $-$ corresponds to the left and right surface states, respectively. We can see that every state in the gap (M, N) has a velocity parallel to a single vector $(Mb, -Nc)$. The current density on each surface carried by the states between E and $E + d\mu$ is then expressed as

$$d\boldsymbol{j}^{\hat{\boldsymbol{x}}} = \mp\frac{e}{h}\left(0, \frac{M}{c}, -\frac{N}{b}\right)d\mu \ \ (\text{at } x = 0, L_x). \quad (11)$$

The derivation of the surface currents on the planes $\perp \hat{\boldsymbol{y}}$ or $\hat{\boldsymbol{z}}$ that contain the conductive axis is slightly different. We consider a finite sample with $0 \leq y \leq L_y, 0 \leq z \leq L_z$. To see which states are mixed, we can write the perturbational term (the off-diagonal term in eq.(7)) for the gap (M, N) in a second quantized form in k space as

$$\mathcal{H}' = \sum_{k_x, k_y, k_z} \Delta e^{i(Mk_yb - Nk_zc)}$$
$$\times c^\dagger_{k_x+MG_b+NG_c, k_y, k_z} c_{k_x, k_y, k_z} + \text{H.c.}, \quad (12)$$

where $c^\dagger(c)$ are creation (annihilation) opperators. In the Wannier representation for y, z, this becomes

$$\mathcal{H}' = \sum_{k_x, m, n} \Delta c^\dagger_{k_x+MG_b+NG_c, m-M, n+N} c_{k_x, m, n} + \text{H.c.}, \quad (13)$$

where $|k_x, m, n\rangle$ is a mixed Wannier-Bloch basis localized at $(y, z) = (mb, nc)$ and delocalized along x (so we call it a 'chain'). Once $\mathcal{H}'$ is switched on, the states at (m, n) with $k_x > 0$ and $(m - M, n + N)$ with $k_x < 0$ are mixed, and an energy gap appears at $k_x = \pm\frac{1}{2}(MG_b + NG_c)$. We can immediately see that chains lying within $M(N)$ lattice constants of the faces $\perp \hat{\boldsymbol{y}}(\hat{\boldsymbol{z}})$ do not couple to other chains, so these states remain gapless, which is exactly the origin of the surface states. The expectation value of the velocity along x is equal to $\pm\frac{\hbar}{2m^*}(MG_b + NG_c)$ with opposite directions between the two sides. The current density for each surface for energies between E and $E + d\mu$ is

$$d\boldsymbol{j}^{\hat{\boldsymbol{y}}} = \pm\frac{e}{h}\left(\frac{M}{c}, 0, 0\right)d\mu \ \ (\text{at } y = 0, L_y),$$

$$d\boldsymbol{j}^{\hat{\boldsymbol{z}}} = \mp\frac{e}{h}\left(\frac{N}{b}, 0, 0\right)d\mu \ \ (\text{at } z = 0, L_z). \quad (14)$$

From eqs.(11),(14), we can see that the currents satisfy Kirchhoff's law on each edge of the sample, so that we end up with a current sheet that *wraps* the whole surface (Fig.1(b)), and the corresponding loop current segment defined above is $d\boldsymbol{j}^{\text{loop}} = \frac{e}{h}\left(0, \frac{N}{b}, \frac{M}{c}\right)d\mu$. We can see that this result is consistent with the formula(4), since the reciprocal vector $\boldsymbol{J}$ (eq.(2)), calculated originally by Montambaux and Kohmoto[5], is $(0, -2\pi N/b, -2\pi M/c)$ for the present case.

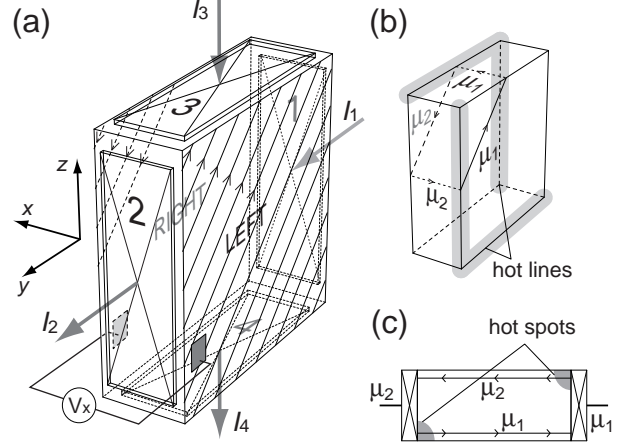
FIG. 3. (a)The experimental setup to detect 3D QHE surface currents. The arrows represent the direction of the currents, which is opposite to the motion of electrons. (b)The "hot line" in the 3D QHE experiment with (c)the corresponding picture in 2D.

In the 3D QHE system, how to measure the conductivity tensor experimentally is even less trivial than in 2D. We propose here an experiment to detect 3D QHE surface currents in analogy with the 2D Hall bar experiment. As shown in Fig.3 we attach two pairs of electrodes, $(1, 2) \perp \hat{\boldsymbol{y}}$ and $(3, 4) \perp \hat{\boldsymbol{z}}$. The incoming or outgoing currents, denoted as $I_1, \cdots, I_4$ as depicted in the figure, are a function of the chemical potentials of the electrodes, $\mu_1, \cdots, \mu_4$. We can calculate the currents by first assuming that all the currents are carried by the surface states. For the present electrodes, we are left with the surface currents on the two $\hat{\boldsymbol{x}}$ faces (which we call right and left surfaces), whose current density is given in eq.(11).

As for the chemical potential, let us consider the situation where all μ's are in the gap (M, N) with $M, N > 0$. Then we can see from eq.(11) that the electrons on the left surface flow from the electrode 1 or 3 (source) into 2 or 4 (drain) with a reverse current for the right surface. So when we set $\mu_1 = \mu_3 \neq \mu_2 = \mu_4$, each $\hat{\boldsymbol{x}}$ face should be in equilibrium with the source electrode (μ_1 for the left surface, μ_2 for the right) if we neglect dissipations in the sample (which we will touch upon later). The net currents must be conserved, which implies, for rectangular surfaces, $I_1 = I_2 (\equiv I_y)$ and $I_3 = I_4 (\equiv -I_z)$, and they are readily calculated, via eq.(11), as

$$(I_y, I_z) = \frac{e}{h} \left(-\frac{L_z M}{c}, \frac{L_y N}{b} \right) (\mu_1 - \mu_2). \tag{15}$$

The Hall conductivity tensor due to the surface conduction becomes

$$(\sigma_{xy}^{\text{surface}}, \sigma_{zx}^{\text{surface}}) = -\frac{e^2}{h} \left(\frac{M}{c}, \frac{N}{b} \right), \tag{16}$$

where we have put $\mu_1 - \mu_2 = -eV_x$ with V_x being the Hall voltage. If we compare this with the expression for the bulk conductivity[5], we can establish a relationship for the Hall conductivities, $\sigma_{ij}^{\text{surface}} = \sigma_{ij}^{\text{bulk}}$ in 3D, i.e., the result *does not change whether the currents flow in the bulk or on the surface*. In the usual 2D QHE, Hatsugai[3] shows that $\sigma_{xy}^{\text{surface}} = \sigma_{xy}^{\text{bulk}}$ by identifing the connection between the topological integers for the bulk and the edge states. So the discussion here in terms of the 3D topological numbers shows that this property remarkably extends to 3D.

We can give an intuitive way to understand why surface or bulk does not really matter. Let us start with 2D QHE to consider two possible situations (Fig.4): Case A has an electrostatic-potential gradient over the bulk with the potential drop, eV, assumed to be the same as the chemical potential difference across the two edges. Case B has no potential drop in the bulk while the chemical potentials at two edges, μ_1, μ_2, differ. Physically, the situation is determined by, e.g., how the local equilibrium is achieved by inelastic processes as studied by Ando in a numerical calucation of the potential profile[12]. We can now question how the σ 's in two pictures are connected. If we put $\mu_1 - \mu_2 = eV$, we can envisage that the two cases cross over to each other continuously as in Fig.4. The only assumption is that we can neglect the scattering across the edge states on the two sides. The current in case A can be divided into the bulk current I^{bulk} and edge currents[13]. The edge currents on the left and right edges have opposite directions but the same intensity because the chemical potential at either edge is assumed to have the same energy difference (denoted by μ_0 in the figure) from the Landau level center. In case B, the conduction is entirely due to the edge currents $I_1^{\text{edge}}, I_2^{\text{edge}}$, which are different because $\mu_1 \neq \mu_2$. Since the total current must be preserved as we go from case A to B, we have $I_1^{\text{edge}} - I_2^{\text{edge}} = I^{\text{bulk}}$, which is in fact the equality in question. If we regard the 3D system as a stack of current segments (or 2D Hall "bars") as in Fig.3(b), this argument can be extended, since currents across the adjacent "bars" are absent. Then we reproduces the property $\sigma^{\text{surface}} = \sigma^{\text{bulk}}$.

As a final comment, in the 2D Hall bar geometry it has long been recognized that there are two hot spots where the chemical potential has to drastically drop from μ_1 to μ_2 dissipatively. In our 3D geometry, the hot spots should become two "hot lines" as shown in Fig.3(b).

Given that the required magnetic field (< 40 T) is well within experimental feasibility as estimated in[7,11], experimental detection of the wrapping currents and hot lines should be interesting.
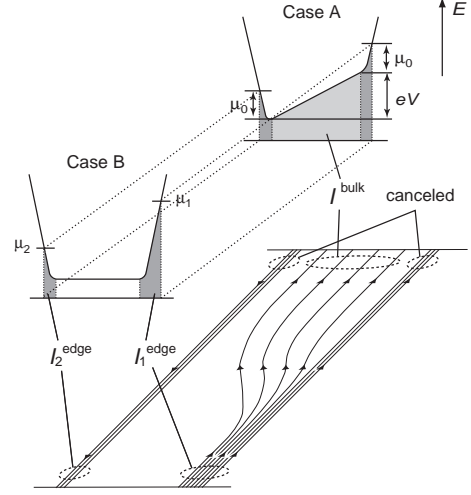
FIG. 4. An intuitive picture which explains the correspondence σ^{surface} and σ^{bulk} in the 2D Hall bar.

[1] B. I. Halperin, Phys. Rev. B **25** 2185 (1982)

[2] H. Aoki and T. Ando, Solid State Commun. **38**, 1079 (1981).

[3] Y. Hatsugai, Phys. Rev. Lett. **71** 3697 (1993).

[4] B. I. Halperin, Jpn. J. Appl. Phys. Suppl. **26**, 1913 (1987).

[5] G. Montambaux and M. Kohmoto, Phys. Rev. B **41**, 11417 (1990).

[6] M. Kohmoto, B. I. Halperin, and Y. Wu, Phys. Rev. B **45**, 13488 (1992).

[7] M. Koshino, H. Aoki, K. Kuroki, S. Kagoshima, and T. Osada, Phys. Rev. Lett. **86**, 1062 (2001); Phys. Rev. B **65**, 045310 (2002).

[8] L. Balents and M. P. A. Fisher, Phys. Rev. Lett. **76**, 2782 (1996).

[9] V. M. Yakovenko, and H.-S. Goan, J. Phys. (France) I **6**, 1917 (1996).

[10] K. Sengupta, H.-J. Kwon, and V. M. Yakovenko, Phys. Rev. Lett. **86**, 1094 (2001).

[11] M. Koshino, H. Aoki, and T. Osada, Phys. Rev. B, to be published.

[12] T. Ando, Surface Science **361/362**, 270 (1996).

[13] S. Komiyama and H. Hirai, Phys. Rev. B **54**, 2067 (1996).